Symmetry breaking and fluctuations within stochastic mean-field dynamics: importance of initial quantum fluctuations

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Dynamics of spontaneous symmetry breaking and fluctuations in the Lipkin-Meshkov-Glick model are investigated in a stochastic mean-field approach. Different from the standard mean-field, in the stochastic approach, initial state fluctuations, are incorporated. In weak coupling, the approach perfectly reproduces the exact quantal dynamics. On the other hand, for increasing coupling strength, above the symmetry breaking threshold, the approach provides description of gross properties (i.e. time averaged behavior) of the exact quantal evolution.

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The mean-field description of a many-body system, i.e. the Hartree-Fock (HF) and/or time-dependent Hartree-Fock theory (TDHF), provides a simple tool for descriptions of certain aspects of complex quantum systems [1]. For example, in the constrained Hartee-Fock method, by explicitly breaking certain symmetries of the underlying Hamiltonian in static calculation, it is possible to describe topology of a quantum phase transitions [2]. However, it is well-known that the mean-field approximation is suitable for the description of mean values of one-body observables, while quantum fluctuations of collective variables are severely underestimated [3]. Numerous approaches have been proposed either deterministic or stochastic to extended mean-field and describe fluctuations in collective space [4, 5]. Most often, these approaches are too complex to be applied in realistic situations with actual computational power. A second limitation of mean-field dynamics is that it can not describe spontaneous symmetry breaking during dynamical evolution. If certain symmetries are present in the initial state, these symmetries are preserved during the evolution [1, 2]. Accordingly, mean-field cannot describe physical effects related to spontaneous symmetry breaking including molecule dissociation, spontaneous magnetization, and spontaneous fission in nuclei.

Both dynamical symmetry breaking and lack of fluctuations are related to the absence of quantal effects in collective space and consequently collective motion appears nearly classical in the mean-field dynamics. To overcome this difficulty, the mean-field approximation should be improved by considering a more general wave function by coherent superposition of Slater determinants, such as in the time-dependent generator coordinate method [6, 7]. However, at present, applications of this method can be made only in a very restricted collective space and mostly along the adiabatic potential energy surface. Here, we employ a stochastic approach, which is much simpler than the generator coordinate method, and is based on the fact that initial state fluctuations (quantal and thermal) dominate the fluctuation dynamics at low energies [8, 9]. This idea has been proposed nearly 30 years ago by Esbensen et al. in a macroscopic model of nuclear reactions [10, 11], and more recently tested in heavy-ion fusion reactions [12]. Following a similar idea, recently, a stochastic mean-field approach (SMF) has been proposed [13] to treat fluctuations beyond mean-field description. In the standard mean-field dynamics, ignoring quantal and thermal fluctuations, the initial state is specified in a deterministic manner: a given initial state leads to a well defined final outcome. In the SMF, on the other hand, initial state fluctuations are incorporated in a stochastic approximation. Consequently, an ensemble of events are generated starting from a specified distribution of initial states. It is shown in ref. [13], in small amplitude limit, that this approach gives rise to the same expression for dispersions of one-body observables as the one obtained in the variational description of Balian and Vénéroni (BV) [14, 15]. In other applications, the average version of SMF theory was recently employed [16–18] to successfully reconcile onset of dissipation in TDHF and to calculate transport coefficients for relative momentum and nucleon-exchange in deep-inelastic heavy-ion collisions [19].

Recently, the variational approach of BV has been applied to nuclear reactions [20, 21]. Similarly to the standard mean-field description, the approach cannot describe spontaneous symmetry breaking mechanism, unless a symmetry-breaking density is used in the varia-

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tional principle. Therefore, the variational approach can only provide a poor approximation for dynamical evolution in the case of spontaneous symmetry breaking (SSB) (see Figure 6 of ref. [22]). Currently, a realistic description of spontaneous symmetry breaking in the mean-field framework remains an open problem. For this reason it is worthwhile to test whether the SMF approach overcomes this difficulty. In the SMF approach the initial state is not the standard HF state, but specified by a suitable distribution. Even if the HF state respects a symmetry, in the SMF, this symmetry may be broken initially event by event. Consequently one might anticipate that, contrary to the original TDHF and/or BV methods, in the SMF approach it may be possible to treat the onset of the SSB. We illustrate here that this is indeed the case.

As a test case, the Lipkin-Meshkov-Glick (LMG) Model [2, 23–25] is considered here. This model consists of N particles distributed in two N-fold degenerated single-particle states separated by an energy ε. The associated Hamiltonian is given by (taking $\hbar = 1$),

$$H = \varepsilon J_z - V(J_x^2 - J_y^2), \tag{1}$$

where V denotes the interaction strength while J_i ($i = x$, y, z), are the quasi-spin operators defined as

$$\begin{aligned} J_z &= \frac{1}{2}\sum_{p=1}^{N}\left(c^\dagger_{+,p}c_{+,p} - c^\dagger_{-,p}c_{-,p}\right), \\ J_x &= \frac{1}{2}(J_+ + J_-), \quad J_y = \frac{1}{2i}(J_+ - J_-) \end{aligned} \tag{2}$$

with $J_+ = \sum_{p=1}^{N} c^\dagger_{+,p}c_{-,p}$, $J_- = J_+^\dagger$ and where $c^\dagger_{+,p}$ and $c^\dagger_{-,p}$ are creation operators associated with the upper and lower single-particle levels. In the following, energies and times are given in ε and $\hbar/\varepsilon$ units respectively.

This model has the advantage to be exactly solvable both in the static [2] and dynamical case [26, 27]. The LMG model is known to present a spontaneous symmetry breaking in mean-field theory as the interaction V increases (see Figure 1 below). Therefore, this model is perfectly suitable to investigate if the SMF approach is able to treat the SBB.

The Hartree-Fock (or Mean-Field) solution is obtained by introducing the Slater Determinant trial states written as $|\Phi\rangle = \Pi_{p=1}^{N} a^\dagger_{0,p}|-\rangle$, where the HF single-particle states are given by

$$a^\dagger_{0,p} = \cos(\alpha)c^\dagger_{-,p} + \sin(\alpha)e^{i\varphi}c^\dagger_{+,p}. \tag{3}$$

The HF solution is obtained by minimizing the mean-field energy with respect to variables α and φ,

$$\mathcal{E}_{\rm HF}[\alpha,\varphi] = -\frac{\varepsilon N}{2}\left\{\cos(2\alpha) + \frac{\chi}{2}\sin^2(2\alpha)\cos(2\varphi)\right\}, \tag{4}$$

where $\chi = V(N-1)/\varepsilon$. In Fig. 1, $\mathcal{E}_{\rm HF}[\alpha, 0]$ is shown for different χ parameters. When the strength parameter is larger than a critical value ($\chi > 1$), the parity symmetry is broken in α direction.

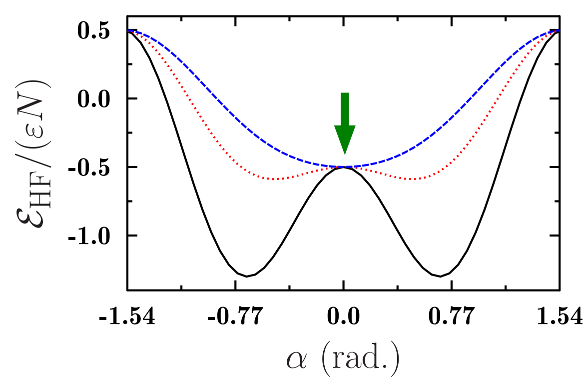

FIG. 1: (color online). Evolution of the Hartree-Fock energy $\mathcal{E}_{\rm HF}$ as a function of α for $\chi = 0.5$ (dashed line), $\chi = 1.8$ (doted line) and $\chi = 5$ (solid line) for $N = 40$ particles. The arrow indicates the initial condition used in the SMF dynamics.

The mean-field evolution can be formulated either in the Schrödinger [27] or Heisenberg picture. Here, we employ the second option. We consider the expectation values of the quasi-spin operators $j_i \equiv \langle J_i \rangle / N$ (for $i = x$, y and z). In the mean-field approximation, it is possible to derive a set of coupled equations for the expectation values of the quasi-spin operators as,

$$\frac{d}{dt}\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \varepsilon \begin{pmatrix} 0 & -1+\chi j_z & \chi j_y \\ 1+\chi j_z & 0 & \chi j_x \\ -2\chi j_y & -2\chi j_x & 0 \end{pmatrix}\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix}. \tag{5}$$

Initially, we prepare the system in the state $|j, -j\rangle$, i.e. $\alpha = 0$, which means that all particles are placed in the lower single-particle states. This case is indicated by an arrow in Figure 1. In this state, initial expectation values of quasi-spin components are $j_z(t_0) = -1/2$, $j_x(t_0) = j_y(t_0) = 0$. This initial condition is a stationary solution of Eq. (5). When the strength parameter is larger that critical value $\chi > 1$, the initial state is at the saddle point. Since mean-field cannot break the symmetry, the system will remain at the saddle point. Therefore, it is not possible to describe onset of SSB in the standard mean-field framework. This situation is similar to the classical object positioned at $\alpha = 0$. In exact quantal description, since the initial state is not an eigenstate of the Hamiltonian H, different spin components and their correlations change in time. The difference between the exact and the mean-field evolution is that quantum fluctuations are properly taken into account in the exact evolution.

In the SMF approach, the expectation values of the quasi-spin operators obey the same set of equations given by Eq. (5), except that the initial conditions are different. In order to simulate quantum fluctuations in an approximate manner, in the SMF approach [13], an initial ensemble of single-particle density matrices is prepared around the same state $|j, -j\rangle$ used in the exact evolution. According to the stochastic properties of the initial

state, it is possible to determine the initial distributions of expectation values of quasi-spin operators. We find that that the z quasi-spin component is not a fluctuating quantity with a mean value $j_z(t_0) = -\frac{1}{2}$. On the other hand, the x and y quasi-spin components are uncorrelated Gaussian random numbers with zero mean values,

$$\overline{j_x^\lambda(t_0)} = \overline{j_y^\lambda(t_0)} = 0, \tag{6}$$

and second moments determined by,

$$\overline{j_x^\lambda(t_0) j_x^\lambda(t_0)} = \overline{j_y^\lambda(t_0) j_y^\lambda(t_0)} = \frac{1}{4N}. \tag{7}$$

We note that even if all trajectories start from the top of the energy landscape (the arrow in Fig. 1) and the system has good parity in average, in the SMF evolution this symmetry is broken event by event due to non-zero values of the spin components along the x and y axis.

In the SMF, mean values and fluctuations of observables are obtained by performing average of expectation values over the generated ensemble. The mean values of the quasi-spin components and associated dispersions, denoted respectively by J_i and Δ_i^2, are given by

$$J_i(t) \;=\; N\overline{j_i^\lambda(t)}, \quad \Delta_i^2(t) = N^2\left(\overline{(j_i^\lambda)^2} - \left(\overline{j_i^\lambda}\right)^2\right). \tag{8}$$

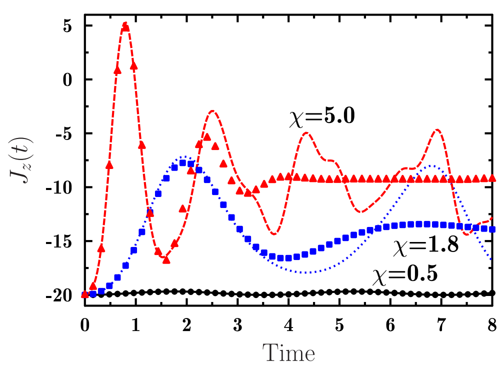

FIG. 2: (color online) Exact evolution of the z quasi-spin component obtained when the initial state is $|j,-j\rangle$ for three different values of χ: $\chi = 0.5$ (solid line), $\chi = 1.8$ (dotted line) and $\chi = 5.0$ (dashed line) for $N = 40$ particles. The corresponding results obtained with the SMF simulations are shown with circles, squares and triangles respectively.

In Fig. 2, the exact and SMF evolutions of the z quasi-spin component obtained when the initial state is $|j,-j\rangle$ for three different values of χ: $\chi = 0.5$, $\chi = 1.8$ and $\chi = 5.0$ are shown. In TDHF, for 40 particles, this component remains constant and equal to -20. In both the exact results and the SMF simulations, mean values of x and y components are zero. In this and following figure, the SMF simulation are carried out using a set of 10^5 trajectories. Simulations are performed using Runge-Kutta or order 2 algorithm with a time step of 0.01.

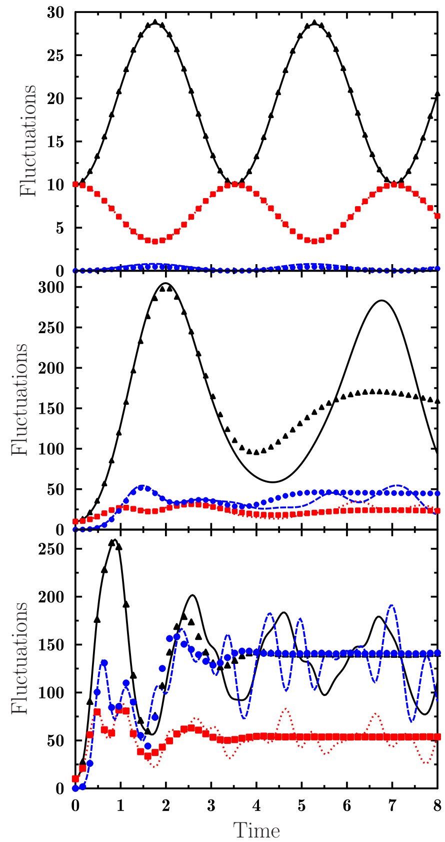

FIG. 3: (color online) Exact evolution of dispersions of quasi-spin operators obtained when the initial state is $|j,-j\rangle$ for three different values of χ, from top to bottom $\chi = 0.5$ (top), $\chi = 1.8$ (middle) and $\chi = 5.0$ (bottom) are shown. In each case, solid, dashed and dotted lines correspond to $\Delta_x^2(t)$, $\Delta_y^2(t)$ and $\Delta_z^2(t)$, respectively. In each case, results of the SMF simulations are shown with triangles (Δ_x^2), squares (Δ_y^2) and circles (Δ_z^2).

The evolutions of dispersions of quasi-spin components obtained in the SMF simulations are shown in Fig. 3, and compared with the exact results, $\Delta_i^2(t) = \langle J_i^2\rangle - \langle J_i\rangle^2$, obtained starting from the state $|j,-j\rangle$. We note that, in the standard TDHF dynamics, since the state $|j,-j\rangle$, does not evolve in time, dispersions of the quasi-spin variables remain constant and equal to their initial values, $\Delta_x^2 = \Delta_y^2 = \frac{N}{4}$ and $\Delta_z^2 = 0$. Below the critical value of the strength parameter ($\chi = 0.5$), where energy can be regarded as nearly harmonic around $\alpha = 0$ (see Figure 1), results obtained in the SMF simulations can hardly be distinguished from the exact solution. Only a small difference is noticeable in the z component. A similar result is obtained in ref. [22] with the BV description. The fact that both approaches produce very similar results in the harmonic limit is not surprising, since it was shown that they both contain the same physical information in this limit [13]. Above the critical strength ($\chi = 1.8$ and 5) (middle and bottom panel of Figure 3), the BV descrip-

tion has been shown to lead to very bad results [22], when calculations start from the same initial condition. Here, we see that the SMF approach provides a fairly good reproduction of gross properties of the exact dynamics. In particular, during the early times, the SMF simulations can not be distinguished from the exact evolution. During the long time evolution, the SMF simulations describe time-averaged behavior of the exact dynamics very well. As seen from Fig. 2, a similar agreement is obtained for the mean value of the z component of quasi-spin for all values of the strength parameter χ. The present example, clearly demonstrates the ability of the SMF approach to describe gross properties of mean values and fluctuations for any strength of the interaction.

It is well known that the standard mean-field theory provides a poor description for fluctuations of collective motion, and it essentially treats the collective motion in a classical approximation. The SMF approach makes an attempt to correct this shortcoming by incorporating quantal and thermal fluctuations in the initial state. In this work, we test the approach in the LMG model. As seen in Fig. 2 and Fig. 3, the SMF simulations provide nearly perfect description for non-trivial oscillations during early evolution of mean values and dispersions of quasi-spin operators. Over the long time interval, simulations also provide a satisfactory description for the gross properties, i.e., time averaged behavior of the mean values and dispersions of quasi-spin operators. We should note that we do not expect that such a simple SMF approach provides a detailed quantum mechanical feature of the evolution. In particular, possible interferences between different trajectories are neglected as well as possible tunneling effects. Nevertheless, the stochastic method presented here provides a suitable framework beyond mean-field for describing dynamics of fluctuations and for understanding spontaneous symmetry breaking in complex quantum systems from a quasi-classical perspective.

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